

Marked-up version of the claims

74. (Amended) A method of identifying a peptide with a predicted indicia of an activity that satisfies a test requirement, comprising the steps of:

[measuring] determining a first indicia of an activity of a plurality of first test peptides from a first test peptide library, wherein the plurality of first peptides is selected using a space-filling technique;

determining a relationship between the [measured] first indicia of the activity and at least one whole molecule parameter of the plurality of first test peptides, wherein the length of said test peptides comprises no greater than twenty amino acids;

determining a test requirement relating to the measured first indicia; and

identifying at least one peptide from a second [test] peptide library containing a plurality of second [test] peptides which based on [the] said relationship, are expected to provide [second] an indicia of [the] activity that satisfies said [meets the] test requirement.

77. (Amended) The method of claim 76, wherein said step of determining a test requirement comprises[the step of determining a]:

quantifying or qualifying the range of [acceptable] an indicia of an [the] activity,

wherein for said activity, the quantified or qualified indicia is greater than the indicia of the first library or less than the indicia of the first library.

78. (Amended) The method of claim 77, wherein said identifying step further comprises:

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determining which of the estimated indicia satisfy [are within] the quantified or qualified range of [acceptable] the indicia; and

determining from the estimated indicia that satisfy [are within] said range, at least one peptide from the plurality of second [test] peptides comprising [from] the second [test] peptide library.

80. (Amended) The method of claim 74, wherein said step of determining a relationship comprises the step of:

determining a distance function $d(x_1, x_2)$ between a first value of a whole molecule parameter, x_1 , of a first test peptide and a second value of the whole molecule parameter, x_2 , of a second [test] peptide not within the first peptide library; and

estimating the indicia of activity of the second [test] peptide as the indicia of the activity of the first peptide if $d(x_1, x_2) \leq d_{\text{cutoff}}$, where d_{cutoff} is a cutoff distance for the first test peptide.

81. (Amended) The method of claim 74, wherein said measuring step is preceded by the step of defining a first test peptide library by representing each of a plurality of groups of peptides as [peptide] isomers from a first peptide space as a respective candidate peptide.

82. (Amended) The method of claim 81, further comprising the step of expanding

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less than all of the candidate peptides determined in said representing step into their constituent compound isomers [peptides] using a space-filling technique.

94. (Amended) The method of claim 74, wherein the first test peptide library consists of peptides having a length [in a range from about] of no less than four amino acids [to about twenty amino acids].

95. (Amended) The method of claim 74, wherein the first test peptide library consists of peptides having a length no more than [in a range from about four amino acids to about] ten amino acids.